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Application No. 09/546,399

Amendment Dated: August 9, 2004

Reply to Office Action mailed April 7, 2004

**Amendments to the Claims:**

1. (Currently Amended). A method for calculating the similarity of at least one chemical compound to at least one chemical probe, comprising the steps of:
  - (a) utilizing at least one chemical descriptor for each of a plurality of compounds, each descriptor comprising a row of a molecule-descriptor matrix  $X$ ;
  - (b) representing each compound as a column of the molecule-descriptor matrix, the entries of the molecule-descriptor matrix comprising a ~~mathematical function of the weighting~~ frequency of each descriptor for each compound;
  - (c) performing a partial singular value decomposition (SVD) of the molecule-descriptor matrix to produce resultant matrices;
  - (d) creating a chemical probe descriptor matrix for the at least one chemical probe, the entries of the chemical probe descriptor matrix comprising a ~~mathematical function of the weighting~~ frequency of each descriptor for each chemical probe;
  - (e) using at least one of the resultant matrices to calculate the similarity between the at least one chemical probe and at least one compound of the molecule descriptor matrix; and
  - (f) providing an output indicating the similarity between the at least one chemical probe and the at least one compound.
2. (Previously Presented). The method as recited in claim 1, wherein each of the at least one chemical descriptors comprise at least one of an atom pair descriptor and a topological torsion descriptor.